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(FILE 'HOME' ENTERED AT 09:36:08 ON 12 APR 2005)

FILE 'REGISTRY' ENTERED AT 09:36:16 ON 12 APR 2005

L1	STRUCTURE UPLOADED
L2	0 S L1
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L4	STRUCTURE UPLOADED
L5	0 S L4 FUL

=>

compounds in spec

SO PCT Int. Appl., 92 pp.

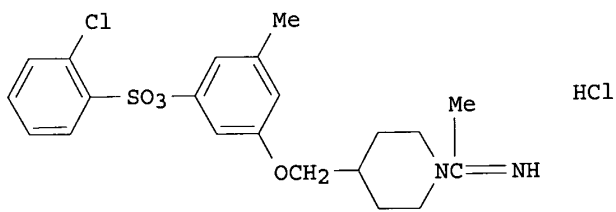
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9724135	A1	19970710	WO 1996-US20087	19961220
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2256309	AA	19970710	CA 1996-2256309	19961220
	AU 9714323	A1	19970728	AU 1997-14323	19961220
	AU 706145	B2	19990610		
	EP 883405	A1	19981216	EP 1996-944847	19961220
	EP 883405	B1	20040225		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	BR 9612360	A	19990713	BR 1996-12360	19961220
	JP 2000503010	T2	20000314	JP 1997-524371	19961220
	AT 260112	E	20040315	AT 1996-944847	19961220
	PT 883405	T	20040630	PT 1996-944847	19961220
	ES 2213786	T3	20040901	ES 1996-944847	19961220
	US 6034127	A	20000307	US 1996-782894	19961227
	NO 9802987	A	19980828	NO 1998-2987	19980626
	US 6133315	A	20001017	US 1999-270734	19990316
	US 6281206	B1	20010828	US 2000-502005	20000211
	US 6225302	B1	20010501	US 2000-631107	20000801
	US 2001025041	A1	20010927	US 2001-851123	20010509
	US 6414020	B2	20020702		
PRAI	US 1995-9431P	P	19951229		
	WO 1996-US20087	W	19961220		
	US 1996-782894	A3	19961227		
	US 1999-270734	A3	19990316		
	US 2000-502005	A3	20000211		
OS	MARPAT 127:135646				
GI					



AB RY(CH₂)_nW(R₁)(CH₂)_mNR₂CR₃:NR₄ [R = substituted Ph; R₁, R₂ = H, alkyl, aralkyl, aryl, hydroxyalkyl, carboxyalkyl; R₁R₂ = bond, CH₂, CH₂CH₂; R₃ = (un)substituted alkyl, cycloalkyl, aryl; R₄ = H, alkyl, OH, alkoxy, aryloxy, aralkoxy, alkoxycarbonyloxy, CN, alkoxycarbonyl, cycloalkoxycarbonyl; W = N, CR₅; R₅ = H, alkyl, aralkyl, aryl, hydroxyalkyl, aminoalkyl, alkylaminoalkyl, dialkylaminoalkyl, carboxyalkyl; Y = O, S, NR₅, CHR₅, bond] were prepared as selective protease

compounds in spec

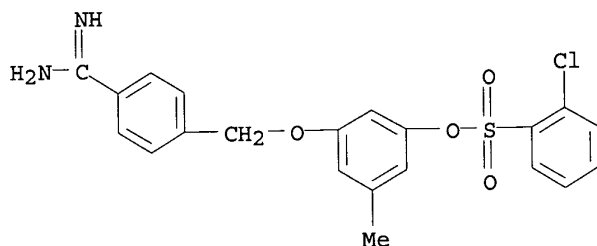
inhibitors, especially for thrombin, factor Xa, trypsin, and chymotrypsin. Thus, isonipectic acid was converted to its N-tert-butoxycarbonyl derivative and reduced to N-tert-butoxycarbonyl-4-piperidinemethanol, which was treated with 2-ClC₆H₄SO₃C₆H₃(OH)Me-3,5, followed by deblocking, reaction with MeC(NH)OEt.HCl to give the imidate I. I had a K_i for thrombin inhibition of 1.65 μM.

IT 193096-44-5P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidine derivs. as selective protease inhibitors)

RN 193096-44-5 CAPLUS

CN Benzenesulfonic acid, 2-chloro-, 3-[[4-(aminoiminomethyl)phenyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L13 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:342428 CAPLUS

DN 126:317391

TI Preparation of [(N-amidinoaziny)alkoxy]phenyl benzenesulfonates and analogs as protease inhibitors

IN Lu, Tianbao; Illig, Carl R.; Tomczuk, Bruce E.; Soll, Richard M.; Subasinghe, Nalin L.; Bone, Roger F.

PA 3-Dimensional Pharmaceuticals, Inc., USA

SO PCT Int. Appl., 144 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	WO 9711693	A1	19970403	WO 1996-US15609	19960927
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI				
	US 5792769	A	19980811	US 1996-698401	19960815
	AU 9672012	A1	19970417	AU 1996-72012	19960927
	AU 714292	B2	19991223		
	EP 859607	A1	19980826	EP 1996-933186	19960927
	EP 859607	B1	20021218		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

compounds in spec

BR 9610876	A	19990713	BR 1996-10876	19960927
JP 11512722	T2	19991102	JP 1996-513732	19960927
NZ 319474	A	20000128	NZ 1996-319474	19960927
AT 229800	E	20030115	AT 1996-933186	19960927
NO 9801393	A	19980525	NO 1998-1393	19980327
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US 1996-698401	A	19960815		
WO 1996-US15609	W	19960927		

OS MARPAT 126:317391

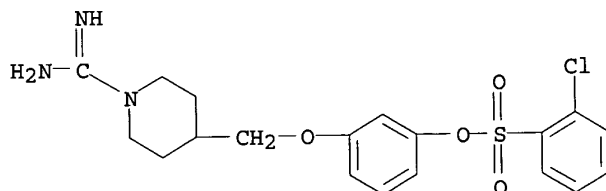
AB R1ZZ1Z2(CH2)nZ3(CH2)mNR8C(:NRa)NRbRc [I; R1 = alk(en)yl, aryl(alkyl), heteroaryl, etc.; Z = NR10SO2, SO2O, NR10CO, etc.; Z1 = (un)substituted phenylene; Z2 = bond, O, S, (alkyl)imino, alkylidene, etc.; Z3 = NR7 or CR7R10; R7,R8 = H, alkyl, aryl(alkyl), etc.; R7R8 = bond, CH2, CH2CH2; R10 = H, (alkoxy)alkyl, aryl(alkyl), etc.; Ra-Rc = H, OH, cyano, alkyl, alkoxy(carbonyl), etc.; m = 1-5; n = 0-8] were prepared Thus, 3-(HO)C6H4OAc was converted in 2 steps to 3-(HO)C6H4OCH2Ph which was esterified by 2-ClC6H4SO2Cl and the deprotected product etherified by N-tert-butoxycarbonyl-4-piperidinylmethyl methanesulfonate to give, in 2 addnl. steps, 2-ClC6H4SO2OC6H4(OCH2R)-3 (R = 1-amidino-4-piperidinyl). Data for biol. activity of I were given.

IT 189338-84-9P 189338-86-1P 189338-92-9P
 189338-99-6P 189339-01-3P 189339-07-9P
 189339-09-1P 189339-11-5P 189339-13-7P
 189339-14-8P 189339-15-9P 189339-16-0P
 189339-17-1P 189339-18-2P 189339-19-3P
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 189339-42-2P 189339-43-3P 189339-44-4P
 189339-45-5P 189339-46-6P 189339-47-7P
 189339-48-8P 189339-49-9P 189339-50-2P
 189339-51-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of [(N-amidinoaziny)alkoxy]phenyl benzenesulfonates and analogs as protease inhibitors)

RN 189338-84-9 CAPLUS

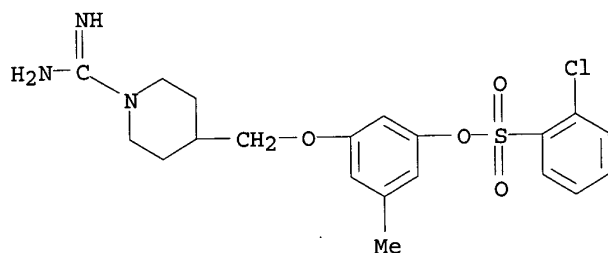
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]phenyl ester (9CI) (CA INDEX NAME)



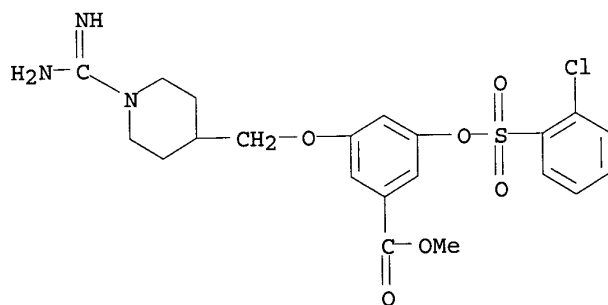
RN 189338-86-1 CAPLUS

CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester (9CI) (CA INDEX NAME)

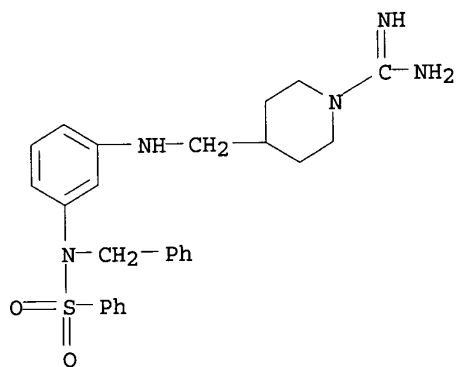
compounds in spec



RN 189338-92-9 CAPLUS
CN Benzoic acid, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-[[2-chlorophenyl)sulfonyl]oxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 189338-99-6 CAPLUS
CN 1-Piperidinecarboximidamide, 4-[[[3-[(phenylmethyl) (phenylsulfonyl) amino]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

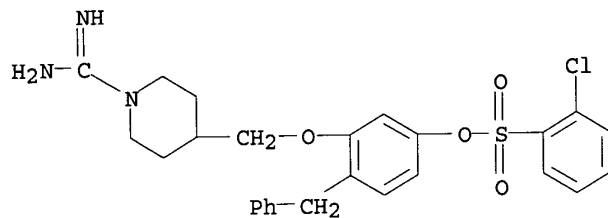


RN 189339-01-3 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-4-(phenylmethyl)phenyl ester, monoacetate (9CI) (CA INDEX NAME)

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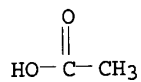
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CMF C26 H28 Cl N3 O4 S

compounds in spec



CM 2

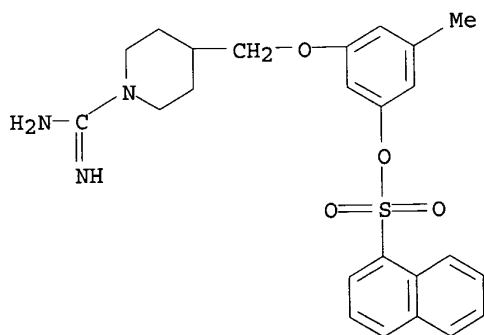
CRN 64-19-7
CMF C2 H4 O2



RN 189339-07-9 CAPLUS
CN 1-Naphthalenesulfonic acid, 3-[[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

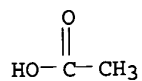
CM 1

CRN 189339-06-8
CMF C24 H27 N3 O4 S



CM 2

CRN 64-19-7
CMF C2 H4 O2



RN 189339-09-1 CAPLUS

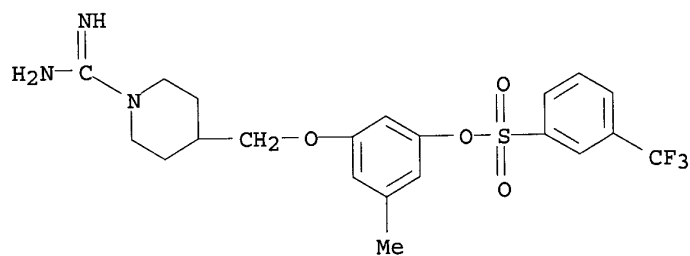
compounds in spec

CN Benzenesulfonic acid, 3-(trifluoromethyl)-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-08-0

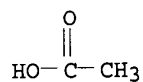
CMF C21 H24 F3 N3 O4 S



CM 2

CRN 64-19-7

CMF C2 H4 O2



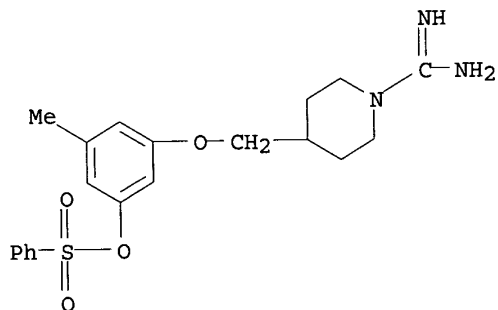
RN 189339-11-5 CAPLUS

CN 1-Piperidinecarboximidamide, 4-[[3-methyl-5-[(phenylsulfonyl)oxy]phenoxy]methyl]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-10-4

CMF C20 H25 N3 O4 S

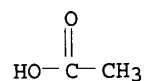


CM 2

CRN 64-19-7

compounds in spec

CMF C2 H4 O2



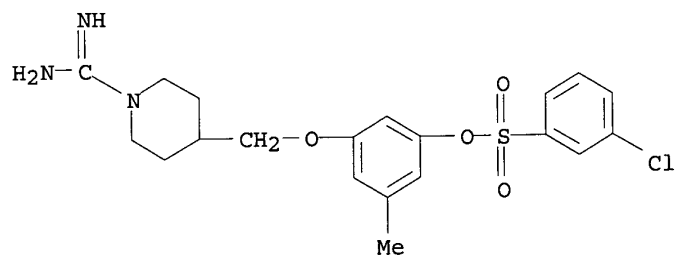
RN 189339-13-7 CAPLUS

CN Benzenesulfonic acid, 3-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-12-6

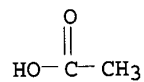
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CM 2

CRN 64-19-7

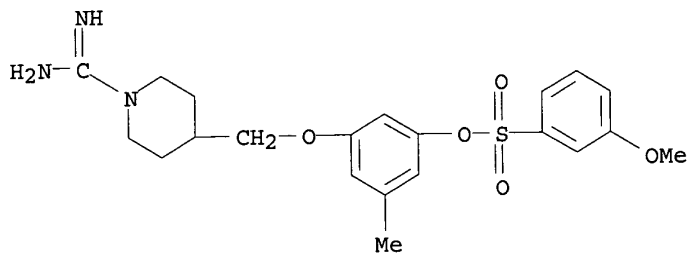
CMF C2 H4 O2



RN 189339-14-8 CAPLUS

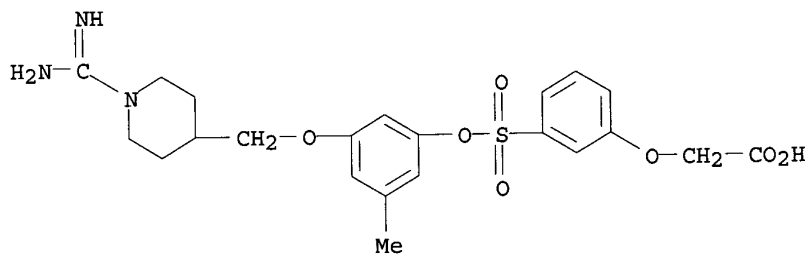
CN Benzenesulfonic acid, 3-methoxy-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

compounds in spec

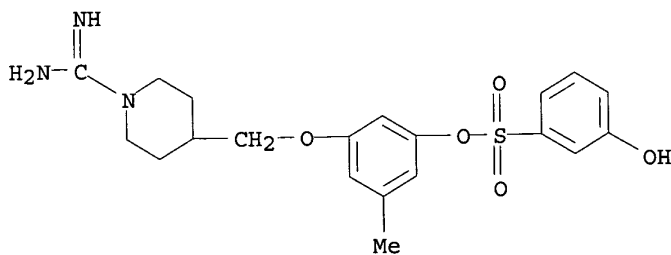


● HCl

RN 189339-15-9 CAPLUS
CN Acetic acid, [3-[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenoxy]sulfonyl]phenoxy]- (9CI) (CA INDEX NAME)



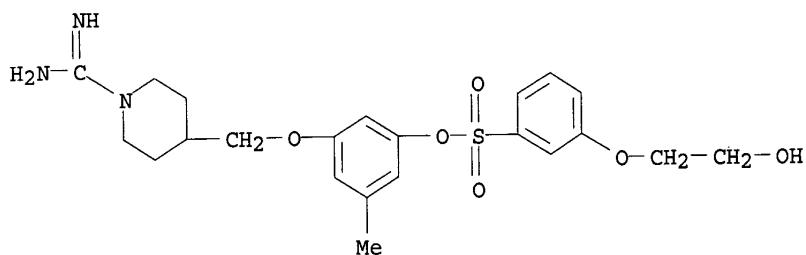
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CN Benzenesulfonic acid, 3-hydroxy-, 3-[[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

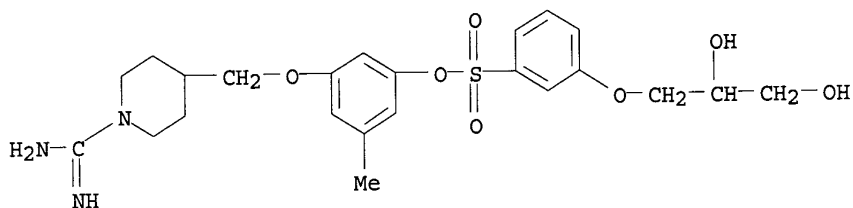
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CN Benzenesulfonic acid, 3-(2-hydroxyethoxy)-, 3-[[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

compounds in spec



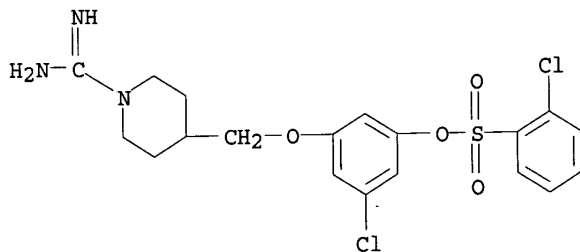
● HCl

RN 189339-18-2 CAPLUS
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● HCl

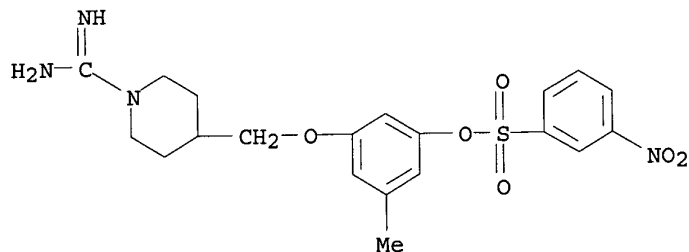
RN 189339-19-3 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-chlorophenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

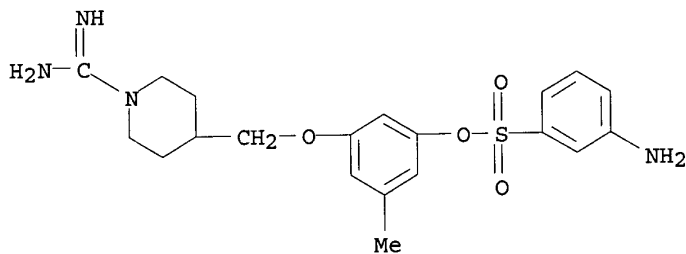
RN 189339-20-6 CAPLUS
CN Benzenesulfonic acid, 3-nitro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

compounds in spec



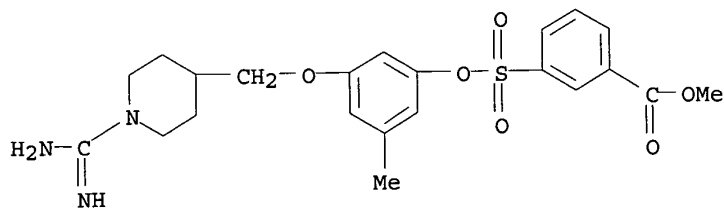
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RN 189339-21-7 CAPLUS
CN Benzenesulfonic acid, 3-amino-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 189339-22-8 CAPLUS
CN Benzoic acid, 3-[[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenoxy]sulfonyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

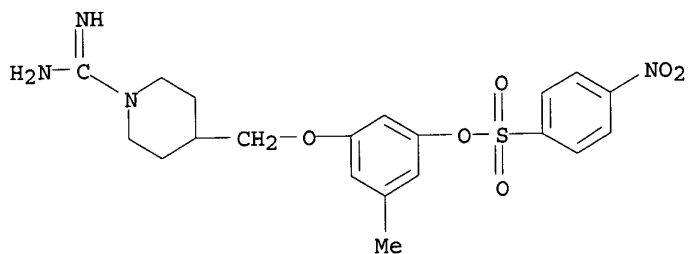


● HCl

RN 189339-23-9 CAPLUS
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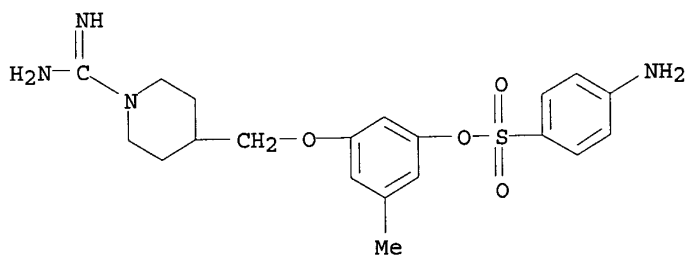
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piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA
INDEX NAME)



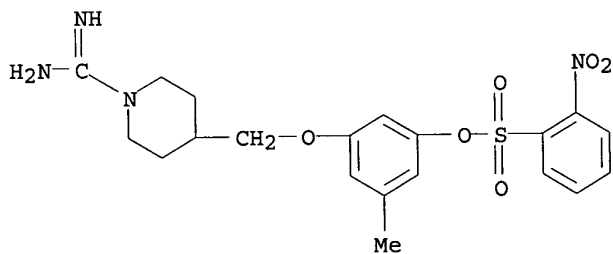
● HCl

RN 189339-24-0 CAPLUS
CN Benzenesulfonic acid, 4-amino-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA
INDEX NAME)



● HCl

RN 189339-25-1 CAPLUS
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INDEX NAME)

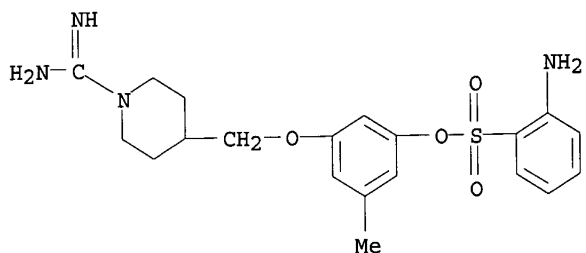


● HCl

compounds in spec

RN 189339-26-2 CAPLUS

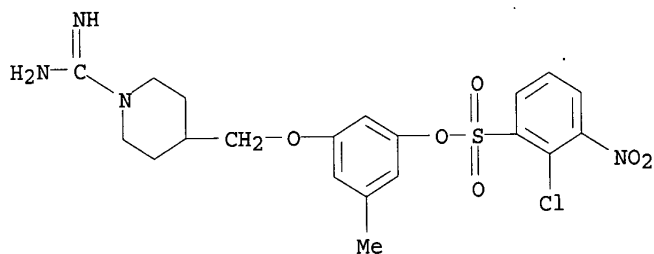
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● HCl

RN 189339-27-3 CAPLUS

CN Benzenesulfonic acid, 2-chloro-3-nitro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

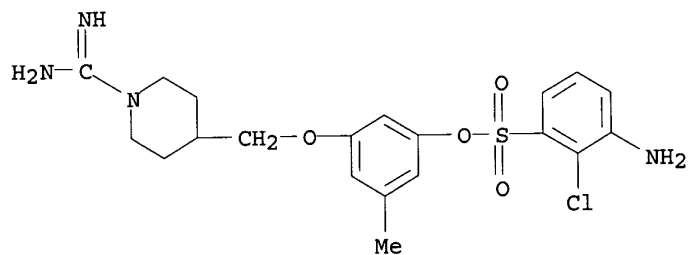


● HCl

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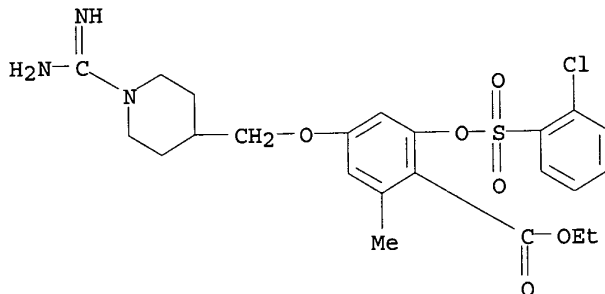
CN Benzenesulfonic acid, 3-amino-2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

compounds in spec



● HCl

RN 189339-29-5 CAPLUS
CN Benzoic acid, 4-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-2-[[2-chlorophenyl)sulfonyl]oxy]-6-methyl-, ethyl ester, monohydrochloride (9CI)
(CA INDEX NAME)



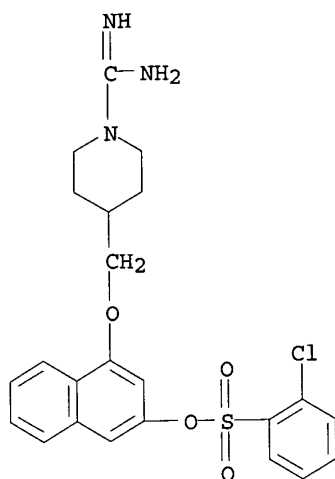
● HCl

RN 189339-31-9 CAPLUS
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CM 1

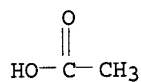
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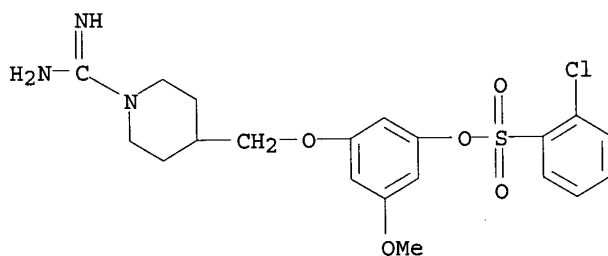


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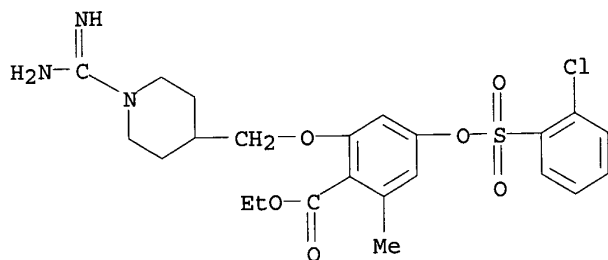


RN 189339-32-0 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methoxyphenyl ester (9CI) (CA INDEX NAME)



RN 189339-33-1 CAPLUS
CN Benzoic acid, 2-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-4-[[2-chlorophenyl)sulfonyl]oxy]-6-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

compounds in spec

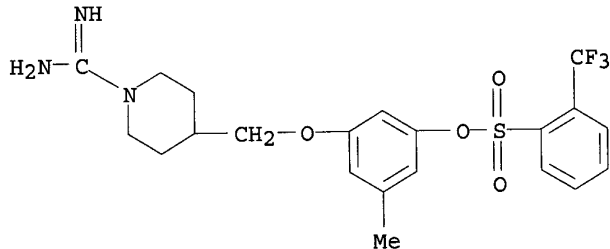


● HCl

RN 189339-35-3 CAPLUS
CN Benzenesulfonic acid, 2-(trifluoromethyl)-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

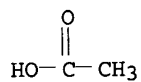
CM 1

CRN 189339-34-2
CMF C21 H24 F3 N3 O4 S



CM 2

CRN 64-19-7
CMF C2 H4 O2

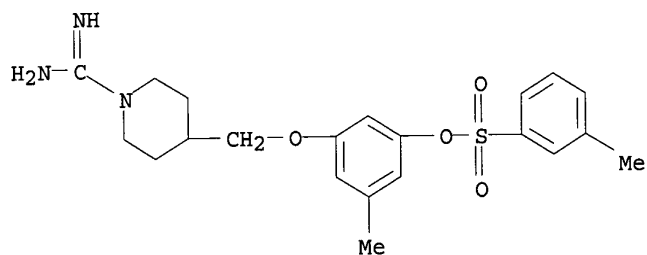


RN 189339-37-5 CAPLUS
CN Benzenesulfonic acid, 3-methyl-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-36-4
CMF C21 H27 N3 O4 S

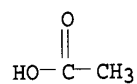
compounds in spec



CM 2

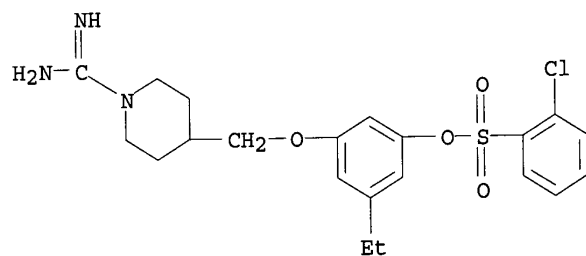
CRN 64-19-7

CMF C2 H4 O2



RN 189339-38-6 CAPLUS

CN Benzenesulfonic acid, 2-chloro-, 3-[[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-ethylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

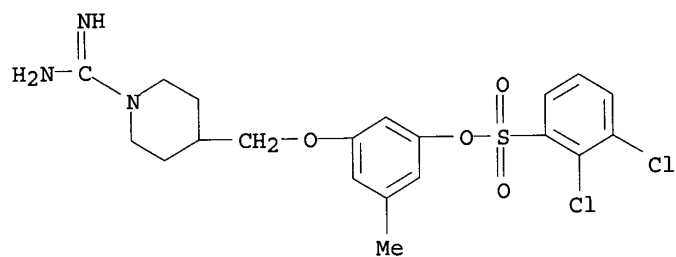


● HCl

RN 189339-40-0 CAPLUS

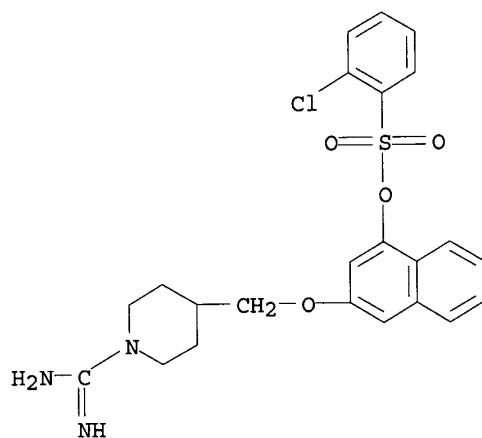
CN Benzenesulfonic acid, 2,3-dichloro-, 3-[[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

compounds in spec



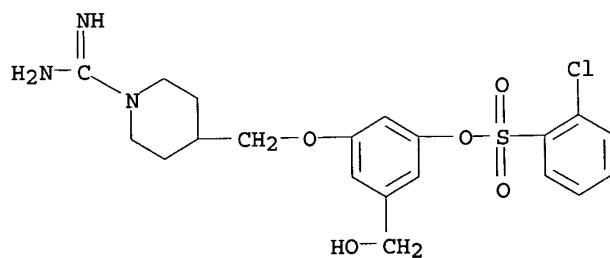
● HCl

RN 189339-41-1 CAPLUS
 CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-1-naphthalenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

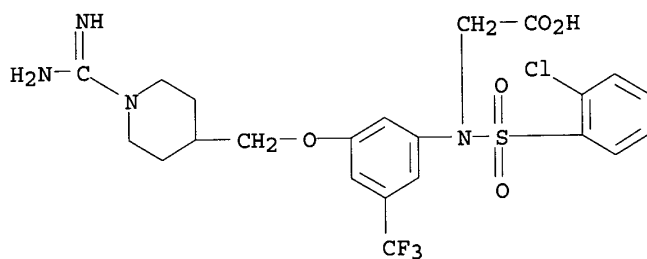
RN 189339-42-2 CAPLUS
 CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-(hydroxymethyl)phenyl ester (9CI) (CA INDEX NAME)



compounds in spec

RN 189339-43-3 CAPLUS

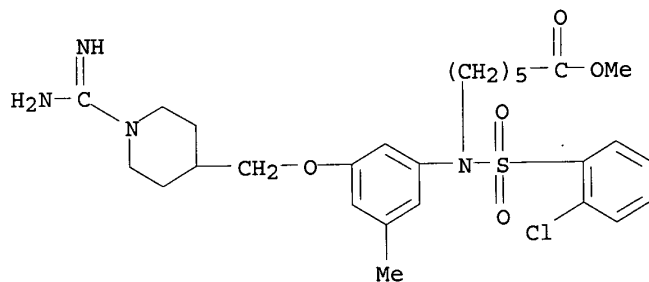
CN Glycine, N-[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-(trifluoromethyl)phenyl]-N-[(2-chlorophenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 189339-44-4 CAPLUS

CN Hexanoic acid, 6-[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl][(2-chlorophenyl)sulfonyl]amino]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

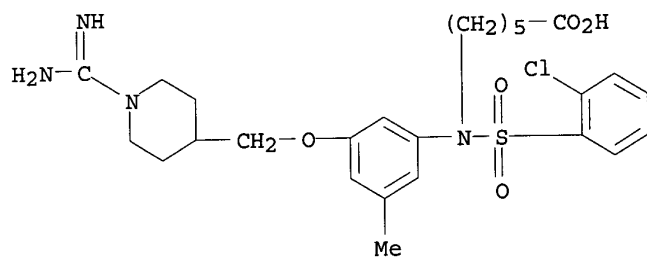


● HCl

RN 189339-45-5 CAPLUS

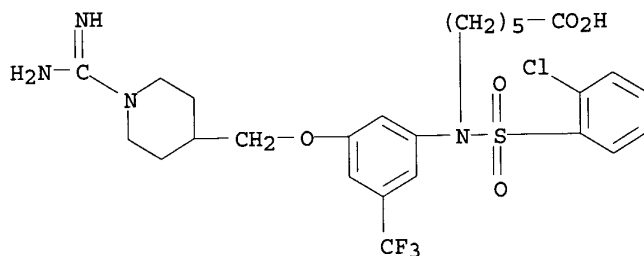
CN Hexanoic acid, 6-[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl][(2-chlorophenyl)sulfonyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

compounds in spec

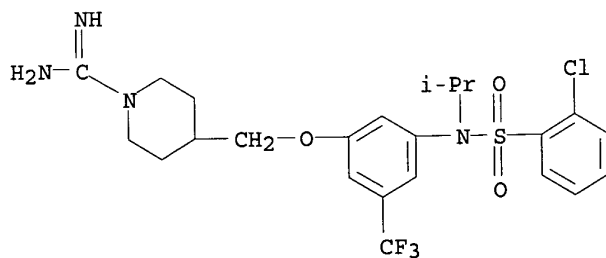


● HCl

RN 189339-46-6 CAPLUS
CN Hexanoic acid, 6-[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-(trifluoromethyl)phenyl][(2-chlorophenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)



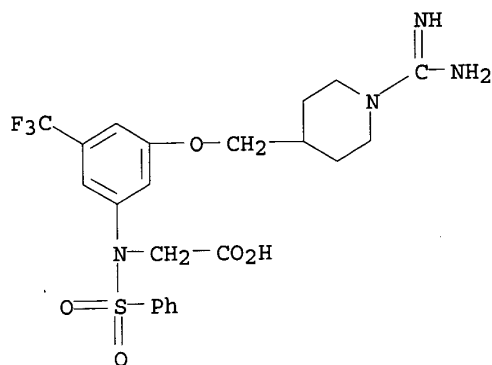
RN 189339-47-7 CAPLUS
CN 1-Piperidinecarboximidamide, 4-[[3-[[2-chlorophenyl)sulfonyl](1-methylethyl)amino]-5-(trifluoromethyl)phenoxy]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

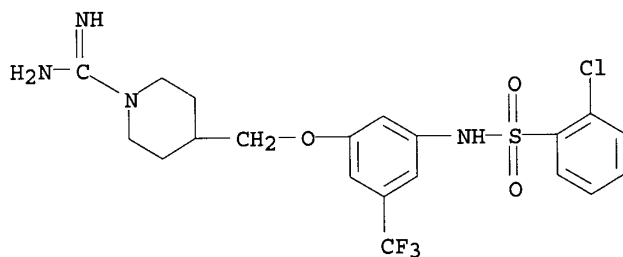
RN 189339-48-8 CAPLUS
CN Glycine, N-[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-(trifluoromethyl)phenyl]-N-(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

compounds in spec



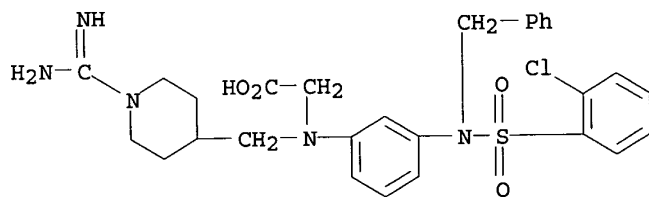
● HCl

RN 189339-49-9 CAPLUS
CN 1-Piperidinecarboximidamide, 4-[[3-[[[(2-chlorophenyl)sulfonyl]amino]-5-(trifluoromethyl)phenoxy]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



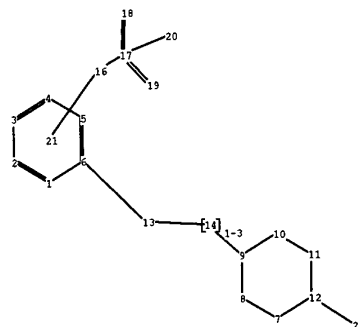
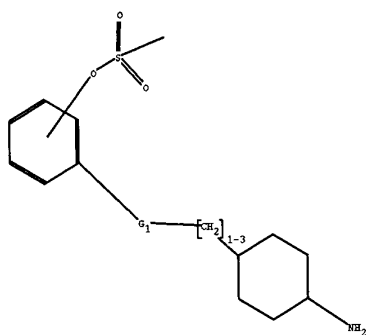
● HCl

RN 189339-50-2 CAPLUS
CN Glycine, N-[[1-(aminoiminomethyl)-4-piperidinyl]methyl]-N-[3-[[[(2-chlorophenyl)sulfonyl] (phenylmethyl)amino]phenyl]- (9CI) (CA INDEX NAME)



RN 189339-51-3 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-[imino[(methoxycarbonyl)amino]methyl]-4-piperidinyl]methoxy]-5-methylphenyl ester (9CI) (CA INDEX NAME)

C:\Program Files\Stnexp\Queries\lat2.str



chain nodes :

13 14 16 17 18 19 22

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

20

chain bonds :

6-13 9-14 12-22 13-14 16-17 17-18 17-19 17-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

6-13 7-8 7-12 8-9 9-10 10-11 11-12 12-22 13-14 16-17 17-18 17-19 17-20

exact bonds :

9-14

normalized bonds :

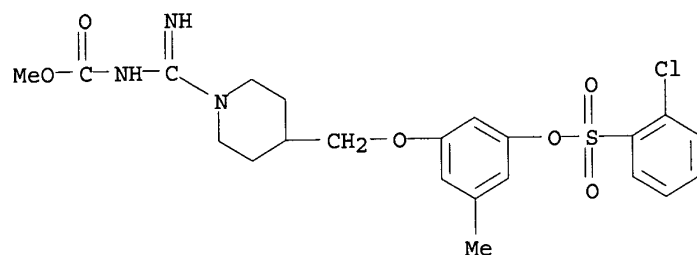
1-2 1-6 2-3 3-4 4-5 5-6

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS

compounds in spec



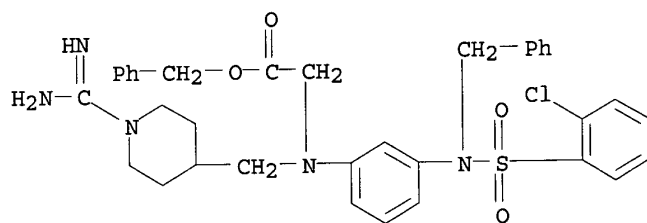
IT **189341-58-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [(N-amidinoaziny)alkoxy]phenyl benzenesulfonates and analogs as protease inhibitors)

RN 189341-58-0 CAPLUS

CN Glycine, N-[[1-(aminoiminomethyl)-4-piperidiny]methyl]-N-[3-[[2-chlorophenyl)sulfonyl](phenylmethyl)amino]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



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